

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 8.19e-02

Global applicability domain: Inside

Local applicability domain index: 5.72e-01

Confidence level: 8.05e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Acrolein</div> <div>Measured: -0.0100</div> <div>Predicted: 8.19e-02</div>	<div>Image not found</div> <div>1-Propyne</div> <div>Measured: 0.94</div> <div>Predicted: 1.01</div>	<div>Image not found</div> <div>Propargyl alcohol</div> <div>Measured: -0.380</div> <div>Predicted: -0.333</div>
<div>Image not found</div> <div>3-Furanmethanol</div> <div>Measured: 0.3</div> <div>Predicted: -0.130</div>	<div>Image not found</div> <div>Furfuryl alcohol</div> <div>Measured: 0.28</div> <div>Predicted: -0.346</div>	